



Carbon in GaN (J. Lyons and A. Janotti)

## Materials 279-Winter 2014

### First-principles Calculations for Materials

Time: Tu-Th 11:00-12:15. Location: Eng II 1355

#### Instructor

- [Prof. Chris G. Van de Walle](#)
- Email: [vandewalle@mrl.ucsb.edu](mailto:vandewalle@mrl.ucsb.edu)
- Office: Eng II 2510
- Office Hours: by appointment

#### Readers

- Luke Gordon, [lukegordon@engineering.ucsb.edu](mailto:lukegordon@engineering.ucsb.edu)
- Lars Bjaalie, [bjaalie@gmail.com](mailto:bjaalie@gmail.com)

**Textbook:** *Electronic Structure: Basic Theory and Practical Methods*, by Richard M. Martin (Cambridge University Press, 2004).

More information about the book, errata, etc, at <http://electronicstructure.org/>

**Goals:** Density-functional theory has made it possible to calculate properties of materials directly from the fundamental equations for the electrons, providing new insights into critical problems in physics, chemistry, and materials science. This course will cover the basic theory and methods of electronic structure, illustrated with examples of practical computational methods and real-world applications. We will discuss the fundamentals (referring back to original papers), practical implementations, and limitations.

**Topics:** Band structure of solids; Uniform electron gas and simple metals; Foundations of density functional theory; Exchange and correlation functionals; Solution of the Kohn–Sham equations; Pseudopotentials; Plane wave basis sets; Tight binding; Augmented functions; Quantum molecular dynamics; Response functions; Excitation spectra; Optical properties; Predicting materials properties: bulk, surfaces, interfaces, defects.

#### Grading:

- |   |     |
|---|-----|
| • Assignments   | 30% |
| – Practicing methodology  |     |
| – Research specific topics  |     |
| • Project   | 40% |
| • Final   | 30% |
| – Aimed at testing understanding of material  |     |
| » While listening/studying/reading, ask yourself: would I be able to explain this to somebody else? |     |

---

---

## Announcements:

- Eq. (3.1) in the textbook has a sign error in the second term of the Hamiltonian: it should have a minus sign.
- Please use descriptive file names for the documents (doc or pdf) that you submit for assignments; e.g., "Assignment 2-lastname.doc".

## Lecture notes:

Tuesday January 7: [Introduction](#)

Thursday January 9: [Introduction \(2\)](#): Ch. 1; Basic Equations: Ch. 3 pp. 52-53

Tuesday January 14: Basic Equations: pp. 53-58 (top); 59 (Theory students only); 61.

Thursday January 16: Basic Equations: pp. 63-64; 65-68 (Koopmans' theorem and Sec. 3.6: Theory students only); Homogeneous electron gas: Ch. 5 pp. 100-102

## Read ahead:

Periodic solids and electron bands: Ch. 4, Secs. 4.1, 4.2: review; Secs. 4.3-4.7 (not p. 90).

Homogeneous electron gas: Ch. 5 pp. 102-112 (not: Density Matrix, p. 103; p. 105, bottom (after Eq. 5.14) and 106, top)

## Assignments:

[Assignment 1](#). Due Thursday January 16, 5 pm, by email to [lukegordon@engineering.ucsb.edu](mailto:lukegordon@engineering.ucsb.edu)

[Assignment 2](#). Due Thursday January 23, 5 pm, by email to [lukegordon@engineering.ucsb.edu](mailto:lukegordon@engineering.ucsb.edu)

[Assignment 3](#). Due Thursday January 30, 5 pm, by email to [lukegordon@engineering.ucsb.edu](mailto:lukegordon@engineering.ucsb.edu)

## Additional assignments for the Theory students in the class:

Jan. 9: Read Appendix C; Appendix F, pp. 499-504.

## Solutions Assignments:

## Final projects:

## Final: